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PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

\* \* \* \* \* Welcome to STN International \* \* \* \* \*

NEWS	1		Web Page for STN Seminar Schedule - N. America
NEWS	2	MAY 01	New CAS web site launched
NEWS	3	MAY 08	CA/CAPLUS Indian patent publication number format defined
NEWS	4	MAY 14	RDISCLOSURE on STN Easy enhanced with new search and display fields
NEWS	5	MAY 21	BIOSIS reloaded and enhanced with archival data
NEWS	6	MAY 21	TOXCENTER enhanced with BIOSIS reload
NEWS	7	MAY 21	CA/CAPLUS enhanced with additional kind codes for German patents
NEWS	8	MAY 22	CA/CAPLUS enhanced with IPC reclassification in Japanese patents
NEWS	9	JUN 27	CA/CAPLUS enhanced with pre-1967 CAS Registry Numbers
NEWS	10	JUN 29	STN Viewer now available
NEWS	11	JUN 29	STN Express, Version 8.2, now available
NEWS	12	JUL 02	LEMBASE coverage updated
NEWS	13	JUL 02	LMEDLINE coverage updated
NEWS	14	JUL 02	SCISEARCH enhanced with complete author names
NEWS	15	JUL 02	CHEMCATS accession numbers revised
NEWS	16	JUL 02	CA/CAPLUS enhanced with utility model patents from China
NEWS	17	JUL 16	CAPLUS enhanced with French and German abstracts
NEWS	18	JUL 18	CA/CAPLUS patent coverage enhanced
NEWS	19	JUL 26	USPATFULL/USPAT2 enhanced with IPC reclassification
NEWS	20	JUL 30	USGENE now available on STN
NEWS	21	AUG 06	CAS REGISTRY enhanced with new experimental property tags
NEWS	22	AUG 06	BEILSTEIN updated with new compounds
NEWS	23	AUG 06	FSTA enhanced with new thesaurus edition
NEWS	24	AUG 13	CA/CAPLUS enhanced with additional kind codes for granted patents
NEWS	25	AUG 20	CA/CAPLUS enhanced with CAS indexing in pre-1907 records
NEWS	26	AUG 27	Full-text patent databases enhanced with predefined patent family display formats from INPADOCDB
NEWS	27	AUG 27	USPATOLD now available on STN
NEWS	28	AUG 28	CAS REGISTRY enhanced with additional experimental spectral property data
NEWS EXPRESS	29	JUNE 2007:	CURRENT WINDOWS VERSION IS V8.2, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 05 JULY 2007.
NEWS HOURS			STN Operating Hours Plus Help Desk Availability
NEWS LOGIN			Welcome Banner and News Items
NEWS IPC8			For general information regarding STN implementation of IPC 8

Enter NEWS followed by the item number or name to see news on that specific topic.

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\* \* \* \* \* STN Columbus \* \* \* \* \*

FILE 'HOME' ENTERED AT 15:57:41 ON 29 AUG 2007

=> FILE REG

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

0.21

0.21

FILE 'REGISTRY' ENTERED AT 15:57:53 ON 29 AUG 2007

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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 28 AUG 2007 HIGHEST RN 945714-55-6

DICTIONARY FILE UPDATES: 28 AUG 2007 HIGHEST RN 945714-55-6

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TSCA INFORMATION NOW CURRENT THROUGH June 29, 2007

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stndoc/properties.html>

=> ....Testing the current file.... screen

ENTER SCREEN EXPRESSION OR (END):end

=> screen 1992 OR 2004 OR 2016 OR 2021 OR 2026

L1 SCREEN CREATED

=>

Uploading C:\Program Files\Stnexp\Queries\10575485.str

L2 STRUCTURE UPLOADED

=> que L2 NOT L1

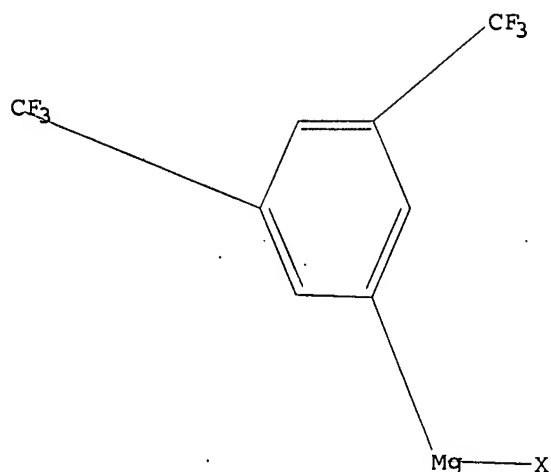
L3 QUE L2 NOT L1

=> D L3

L3 HAS NO ANSWERS

L1 SCR 1992 OR 2004 OR 2016 OR 2021 OR 2026

L2 STR



Structure attributes must be viewed using STN Express query preparation.  
 L3 QUE ABB=ON PLU=ON L2 NOT L1

=> S L3  
 SAMPLE SEARCH INITIATED 15:58:11 FILE 'REGISTRY'  
 SAMPLE SCREEN SEARCH COMPLETED - 0 TO ITERATE

100.0% PROCESSED 0 ITERATIONS 0 ANSWERS  
 SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
 BATCH \*\*COMPLETE\*\*  
 PROJECTED ITERATIONS: 0 TO 0  
 PROJECTED ANSWERS: 0 TO 0

L4 0 SEA SSS SAM L2 NOT L1

=> S L3 FULL  
 FULL SEARCH INITIATED 15:58:16 FILE 'REGISTRY'  
 FULL SCREEN SEARCH COMPLETED - 9 TO ITERATE

100.0% PROCESSED 9 ITERATIONS 2 ANSWERS  
 SEARCH TIME: 00.00.01

L5 2 SEA SSS FUL L2 NOT L1

=> FILE CAPLUS  

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	172.10	172.31

FILE 'CAPLUS' ENTERED AT 15:58:21 ON 29 AUG 2007  
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FILE COVERS 1907 - 29 Aug 2007 VOL 147 ISS 10  
FILE LAST UPDATED: 28 Aug 2007 (20070828/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

<http://www.cas.org/infopolicy.html>

=> S L5

L6 39 L5

=> S PARAFORMALDEHYDE

17521 PARAFORMALDEHYDE

15 PARAFORMALDEHYDES

L7 17523 PARAFORMALDEHYDE

(PARAFORMALDEHYDE OR PARAFORMALDEHYDES)

=> S L6 AND L7

L8 1 L6 AND L7

=> D BIB ABS HITSTR

L8 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2007 ACS on STN

AN 2005:346966 CAPLUS

DN 142:392168

TI Grignard reaction process for the preparation 3,5-bis(trifluoromethyl)benzyl alcohol from 3,5-bis(trifluoromethyl)phenylmagnesium halides and solid paraformaldehyde

IN Nardello, Alessandro; Pretto, Marisa; Faccin, Andrea

PA Miteni S.p.A., Italy

SO PCT Int. Appl., 14 pp.

CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2005035472	A1	20050421	WO 2003-IT616	20031013
	W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
	RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
	AU 2003279541	A1	20050427	AU 2003-279541	20031013
	EP 1673329	A1	20060628	EP 2003-772649	20031013
	R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, SK			
	US 2007135662	A1	20070614	US 2006-575485	20060707
PRAI	WO 2003-IT616	A	20031013		

OS CASREACT 142:392168

AB A Grignard reaction process for the preparation 3,5-bis(trifluoromethyl)benzyl alc. (I) from 3,5-bis(trifluoromethyl)phenylmagnesium halides [e.g., 3,5-bis(trifluoromethyl)phenylmagnesium bromide] and solid paraformaldehyde is described. I can then be converted into 3,5-bis(trifluoromethyl)benzyl halides [e.g., 3,5-

bis(trifluoromethyl)benzyl bromide] by halogenation with hydrogen halides (e.g., hydrogen bromide).

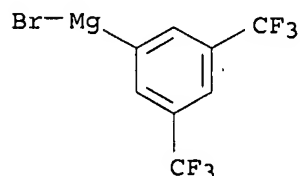
IT 112981-69-8P, 3,5-Bis(trifluoromethyl)phenylmagnesium bromide  
535949-95-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(Grignard reaction process for the preparation 3,5-bis(trifluoromethyl)benzyl alc. from 3,5-bis(trifluoromethyl)phenylmagnesium halides and solid paraformaldehyde)

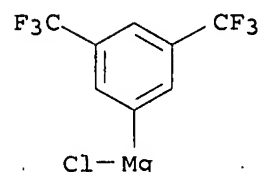
RN 112981-69-8 CAPLUS

CN Magnesium, [3,5-bis(trifluoromethyl)phenyl]bromo- (9CI) (CA INDEX NAME)



RN 535949-95-2 CAPLUS

CN Magnesium, [3,5-bis(trifluoromethyl)phenyl]chloro- (9CI) (CA INDEX NAME)



RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> FILE CASREACT

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

8.69

181.00

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE

TOTAL

ENTRY

SESSION

CA SUBSCRIBER PRICE

-0.78

-0.78

FILE 'CASREACT' ENTERED AT 16:00:00 ON 29 AUG 2007

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FILE CONTENT:1840 - 25 Aug 2007 VOL 147 ISS 10

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\*\*\*\*\*  
\*  
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\*  
\*\*\*\*\*

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This file contains CAS Registry Numbers for easy and accurate substance identification.

=> S L5

L9 16 L5

=> S PARAFORMALDEHYDE

4192 PARAFORMALDEHYDE

1 PARAFORMALDEHYDES

L10 4192 PARAFORMALDEHYDE

(PARAFORMALDEHYDE OR PARAFORMALDEHYDES)

=> S L9 AND L10

L11 1 L9 AND L10

=> D BIB ABS CRDREF

L11 ANSWER 1 OF 1 CASREACT COPYRIGHT 2007 ACS on STN

AN 142:392168 CASREACT

TI Grignard reaction process for the preparation 3,5-bis(trifluoromethyl)benzyl alcohol from 3,5-bis(trifluoromethyl)phenylmagnesium halides and solid paraformaldehyde

IN Nardello, Alessandro; Pretto, Marisa; Faccin, Andrea

PA Miteni S.p.A., Italy

SO PCT Int. Appl., 14 pp.

CODEN: PIXXD2

DT Patent

LA English

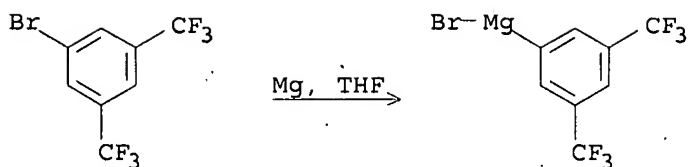
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2005035472	A1	20050421	WO 2003-IT616	20031013
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	RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
	AU 2003279541	A1	20050427	AU 2003-279541	20031013
	EP 1673329	A1	20060628	EP 2003-772649	20031013
	R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, SK			
	US 2007135662	A1	20070614	US 2006-575485	20060707

PRAI WO 2003-IT616 20031013

AB A Grignard reaction process for the preparation 3,5-bis(trifluoromethyl)benzyl alc. (I) from 3,5-bis(trifluoromethyl)phenylmagnesium halides [e.g., 3,5-bis(trifluoromethyl)phenylmagnesium bromide] and solid paraformaldehyde is described. I can then be converted into 3,5-bis(trifluoromethyl)benzyl halides [e.g., 3,5-bis(trifluoromethyl)benzyl bromide] by halogenation with hydrogen halides (e.g., hydrogen bromide).

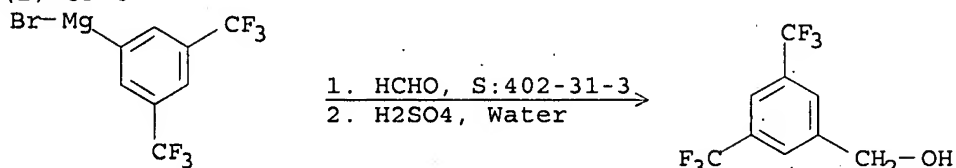
RX(1) OF 6



REF: PCT Int. Appl., 2005035472, 21 Apr 2005

CON: 10 minutes

RX(2) OF 6

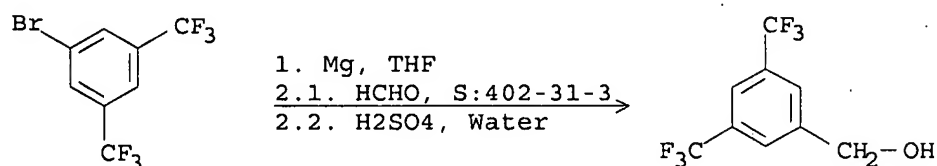


(step 1)

REF: PCT Int. Appl., 14 pp.; 2005

CON: STAGE(1) 6 hours, 45 deg C

RX(4) OF 6 - 2 STEPS

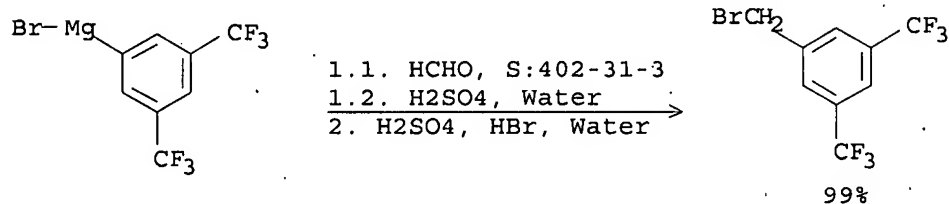


REF: PCT Int. Appl., 14 pp.; 2005

CON: STEP(1) 10 minutes

STEP(2.1) 6 hours, 45 deg C

RX(5) OF 6 - 2 STEPS

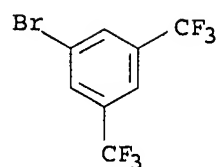


REF: PCT Int. Appl., 14 pp.; 2005

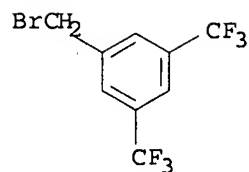
CON: STEP(1.1) 6 hours, 45 deg C

STEP(2.1) 50 deg C; 30 minutes; 100 - 105 deg C; 8 hours;  
1.5 hours, reflux

RX(6) OF 6 - 3 STEPS



1. Mg, THF  
2.1. HCHO, S:402-31-3  
2.2. H<sub>2</sub>SO<sub>4</sub>, Water  
3. H<sub>2</sub>SO<sub>4</sub>, HBr, Water



99%

REF: PCT Int. Appl., 14 pp.; 2005

CON: STEP(1) 10 minutes

STEP(2.1) 6 hours, 45 deg C

STEP(3.1) 50 deg C; 30 minutes; 100 - 105 deg C; 8 hours;  
1.5 hours, reflux

RE.CNT 3

THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT



Searched by Examiner  
Gonzalez

(FILE 'HOME' ENTERED AT 16:11:16 ON 29 AUG 2007)

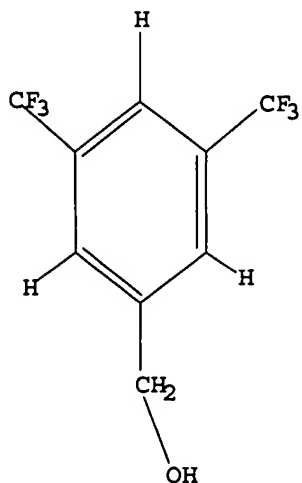
FILE 'REGISTRY' ENTERED AT 16:11:30 ON 29 AUG 2007

L1 STRUCTURE UPLOADED

=> d l1

L1 HAS NO ANSWERS

L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l1

SAMPLE SEARCH INITIATED 16:11:49 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 1126 TO ITERATE

100.0% PROCESSED 1126 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*

BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS: 20507 TO 24533

PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1

=> s l1 full

FULL SEARCH INITIATED 16:11:54 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 22288 TO ITERATE

100.0% PROCESSED 22288 ITERATIONS

1 ANSWERS

SEARCH TIME: 00.00.01

L3 1 SEA SSS FUL L1

=> fil caplus

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

172.10

172.31

FILE 'CAPLUS' ENTERED AT 16:12:00 ON 29 AUG 2007

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FILE COVERS 1907 - 29 Aug 2007 VOL 147 ISS 10  
FILE LAST UPDATED: 28 Aug 2007 (20070828/ED)

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<http://www.cas.org/infopolicy.html>

=> s l1

REGISTRY INITIATED

Substance data SEARCH and crossover from CAS REGISTRY in progress...

Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

SAMPLE SEARCH INITIATED 16:12:03 FILE 'REGISTRY'  
SAMPLE SCREEN SEARCH COMPLETED - 1126 TO ITERATE

100.0% PROCESSED 1126 ITERATIONS  
SEARCH TIME: 00.00.01

0 ANSWERS

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS: 20507 TO 24533  
PROJECTED ANSWERS: 0 TO 0

L4 0 SEA SSS SAM L1

L5 0 L4

=> s l3

L6 57 L3

=> s l3/prep

57 L3

4453515 PREP/RL

L7 9 L3/PREP

(L3 (L) PREP/RL)

=> d 1-9 bib abs

L7 ANSWER 1 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN

AN 2005:346966 CAPLUS

DN 142:392168

TI Grignard reaction process for the preparation 3,5-bis(trifluoromethyl)benzyl alcohol from 3,5-bis(trifluoromethyl)phenylmagnesium halides and solid paraformaldehyde

IN Nardello, Alessandro; Pretto, Marisa; Faccin, Andrea

PA Miteni S.p.A., Italy  
SO PCT Int. Appl., 14 pp.  
CODEN: PIXXD2  
DT Patent  
LA English  
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2005035472	A1	20050421	WO 2003-IT616	20031013
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	AU 2003279541	A1	20050427	AU 2003-279541	20031013
	EP 1673329	A1	20060628	EP 2003-772649	20031013
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, SK				
	US 2007135662	A1	20070614	US 2006-575485	20060707
PRAI	WO 2003-IT616	A	20031013		

OS CASREACT 142:392168

AB A Grignard reaction process for the preparation 3,5-bis(trifluoromethyl)benzyl alc. (I) from 3,5-bis(trifluoromethyl)phenylmagnesium halides [e.g., 3,5-bis(trifluoromethyl)phenylmagnesium bromide] and solid paraformaldehyde is described. I can then be converted into 3,5-bis(trifluoromethyl)benzyl halides [e.g., 3,5-bis(trifluoromethyl)benzyl bromide] by halogenation with hydrogen halides (e.g., hydrogen bromide).

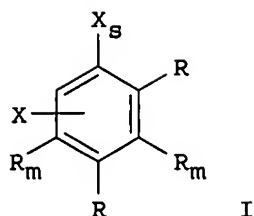
RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 2 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN  
AN 2003:884526 CAPLUS  
DN 139:364696  
TI Preparation of high-purity (fluoroalkyl)benzenes  
IN Hidaka, Toshio; Fushimi, Norio; Yoshimura, Takashi; Kawai, Ken  
PA Mitsubishi Gas Chemical Co., Ltd., Japan  
SO Jpn. Kokai Tokkyo Koho, 14 pp.  
CODEN: JKXXAF

DT Patent  
LA Japanese  
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 2003321406	A	20031111	JP 2002-128158	20020430
	WO 2003093212	A1	20031113	WO 2003-JP5261	20030424
	W: CN, US				
	RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR				
	EP 1500641	A1	20050126	EP 2003-723191	20030424
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, SK				
	CN 1653029	A	20050810	CN 2003-811283	20030424
	US 2006167324	A1	20060727	US 2005-512990	20050616
PRAI	JP 2002-128158	A	20020430		
	WO 2003-JP5261	W	20030424		

OS CASREACT 139:364696; MARPAT 139:364696  
GI



AB Title compds. are prepared by photohalogenation of side chains of alkylbenzenes I (X, X<sub>s</sub> = H, OH, alkyl, aryl, halo, etc.; R, R<sub>m</sub> = H, CO<sub>2</sub>H, halocarbonyl, alkyloxycarbonyl, etc.), showing Group 3-12 transition metal content ≤500 ppm, and treatment with ≥10 mol HF/mol-(haloalkyl)benzene for halogen-F exchange. 2,5-Bis(trichloromethyl)benzoyl chloride (preparation given) was treated with HF at 150° for 13 h to give 83% 3,5-bis(trifluoromethyl)benzoyl fluoride, which was hydrolyzed to give metal-free 3,5-bis(trifluoromethyl)benzoic acid with ≥99.9% purity.

L7 ANSWER 3 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN

AN 2002:361403 CAPLUS

DN 137:279074

TI (S)-(-)- and (R)-(+)-4-methyl-2-hydroxymethyl[2]paracyclo-[2](5,8)quinolinophane: novel N,O-planar chiral catalysts for the enantioselective addition of diethylzinc to aldehydes

AU Ruzziconi, Renzo; Piermatti, Oriana; Ricci, Giacomo; Vinci, Daniele  
CS Dipartimento di Chimica, Universita di Perugia, Perugia, I-6100, Italy

SO Synlett (2002), (5), 747-750  
CODEN: SYNLES; ISSN: 0936-5214

PB Georg Thieme Verlag

DT Journal

LA English

OS CASREACT 137:279074

AB Novel planar chiral N,O-ligands derived from (R)-(+)- and (S)-(-)-2,4-dimethyl[2]paracyclo[2](5,8)quinolinophane were synthesized and employed as catalysts in the enantioselective addition of diethylzinc to aromatic aldehydes. For example, benzaldehyde is alkylated with diethylzinc in the presence of (S)-(-)-4-methyl-2-hydroxymethyl[2]paracyclo-[2](5,8)quinolinophane to give 99% 1-phenyl-1-propanol. On the basis of the ee values, ranging from 30% to 75%, and the configuration of the obtained 1-phenyl-1-propanols, a plausible structure of the transition state for the alkylation process of the aldehydes is discussed.

RE.CNT 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 4 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN

AN 2000:876760 CAPLUS

DN 134:41974

TI Process for the preparation of benzyl alcohols and their use

IN Neugebauer, Torsten; Marhold, Albrecht

PA Bayer A.-G., Germany

SO Eur. Pat. Appl., 8 pp.

CODEN: EPXXDW

DT Patent

LA German

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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PI	EP 1059280	A2	20001213	EP 2000-110999	20000530

EP 1059280 A3 20040204  
 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,  
 IE, SI, LT, LV, FI, RO  
 DE 19926621 A1 20001214 DE 1999-19926621 19990611  
 JP 2001002601 A 20010109 JP 2000-151267 20000523  
 US 6462242 B1 20021008 US 2000-587742 20000605

PRAI DE 1999-19926621 A 19990611  
 OS CASREACT 134:41974; MARPAT 134:41974

AB Benzyl alcs., especially those containing fluoro or fluoroalkyl substituents in the

benzene ring, were prepared by palladium-catalyzed formylation of aryl bromides in the presence of CO and Na formate to give benzaldehydes, followed by reduction of the benzaldehydes with addnl. formate. Thus, 3.62 g 4-CF<sub>3</sub>OC<sub>6</sub>H<sub>4</sub>Br reacted with 1.53 g Na formate and 0.21 g bis(triphenylphosphine)palladium dichloride (I) in 15 mL DMF at 110° with introduction of CO to give a product containing 91% 4-CF<sub>3</sub>OC<sub>6</sub>H<sub>4</sub>CHO (II) and 7% 4-CF<sub>3</sub>OC<sub>6</sub>H<sub>4</sub>CH<sub>2</sub>OH (III). Similarly, 8.55 g II was reduced in the presence of 6.12 g Na formate and 0.63 g I in 45 mL DMF at 110° to give a 69% yield of III.

L7 ANSWER 5 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN  
 AN 1995:482084 CAPLUS  
 DN 122:313954

TI Mechanisms of Benzyl Group Transfer in the Decay of (E)-  
 Arylmethanediazoates and Aryldiazomethanes in Aqueous Solutions

AU Finneman, Jari I.; Fishbein, James C.

CS Department of Chemistry, Wake Forest University, Winston-Salem, NC, 27109, USA

SO Journal of the American Chemical Society (1995), 117(15), 4228-39  
 CODEN: JACSAT; ISSN: 0002-7863

PB American Chemical Society

DT Journal

LA English

AB Rate consts. are reported for the buffer-independent decay of ten (E)-arylmethanediazoates in aqueous media at 25 °, ionic strength 1 M (NaClO<sub>4</sub>), 4% 2-propanol, in the region of pH 4-12. The rate consts. are proportional to hydrogen ion concentration at high pH and become pH independent in the low-pH region. Varying concns. of oxyanion, amine, and hydrazine buffers over the range 0.05-0.2 M increased the pseudo-first-order rate constant for decay of the diazoates by less than 10%. The azide/water selectivities, *k<sub>a</sub>/k<sub>s</sub>*, for partitioning of the benzyl groups in the decay of (E)-(3,5-bis(trifluoromethyl)phenyl)methanediazoate and the (3,5-bis(trifluoromethyl)phenyl)diazomethane are determined to be 0.20 and 0.21 M<sup>-1</sup>, resp., in phosphate buffered water and 0.27 and 0.26 M<sup>-1</sup>, resp., in 20/80 DMSO-water. It is concluded that these two reactants decompose, in these media, via a common free diazonium ion intermediate that is formed in the case of the diazoate upon unassisted N-O bond cleavage of the diazoic acid. A common mechanism is indicated for all the diazoates by the correlation line for the plot of log *k<sub>1</sub>*, the pH independent rate constant, against  $\sigma$  that has a slope  $\rho = -1.23$ . Product ratios for trapping of benzyl groups derived from other pairs of arylmethanediazoates and aryldiazomethanes with less electron withdrawing groups are different outside exptl. error, indicating the importance of different nitrogen-separated ion pairs in these reactions. The (E)-(p-methoxyphenyl)methane-160-diazoate decomps. in 160/180 water to give alc. that has an "excess" abundance of 160 compared to solvent. Decomposition of the same compound in 50/50 trifluoroethanol-water with varying concns. of azide indicates that azide ion appears to trap a limiting amount, .apprx.80%, of the p-methoxybenzyl group. Quant. anal. of the data indicates that 16% of the p-methoxybenzyl cation is trapped by solvent at the nitrogen-separated ion pair stage, in the absence of azide ion. There is a 9-fold enhancement of selectivity for trifluoroethanol at the ion pair stage that is ascribed to a proton switch initiated by the leaving hydroxide ion in the ion pair. The values of *k<sub>a</sub>/k<sub>s</sub>* .apprx. 0.2 M<sup>-1</sup> and

chemical  
kT/kH .apprx. 0.5-0.6 for the trifluoroethanol-water selectivity and  
kET/kT .apprx. 1 for the ethanol-trifluoroethanol selectivity are  
independent of substituent in the decay of arylmethanediazoates (X = H and  
EWG) in water, water-trifluoroethanol (50/50), and water-trifluoroethanol-  
ethanol (50/40/10), resp. The product-determining steps do not involve

bonding but rather rotational/translational reorientation of the  
nucleophiles in the first solvation sphere of the carbocation  
intermediates. The values of kH/kT = 0.5-0.6 indicate preferential  
solvation of the cation precursor by trifluoroethanol. A preferential  
interaction for trifluoroethanol of <1 kcal/mol is required to generate  
the observed selectivities.

L7 ANSWER 6 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN

AN 1985:148404 CAPLUS

DN 102:148404

TI Stereomutation of methoxycarbenium ions. 2. Experimental evidence for an  
inversion process

AU Blackburn, Christopher; Childs, Ronald F.; Cremer, Dieter; Gauss, Juergen  
CS Dep. Chem., McMaster Univ., Hamilton, ON, L8S 4M1, Can.

SO Journal of the American Chemical Society (1985), 107(8), 2442-8  
CODEN: JACSAT; ISSN: 0002-7863

DT Journal

LA English

OS CASREACT 102:148404

AB The stereomutation about the C-O partial double bond of a series of  
1-methoxy- (I) and 1-hydroxy-3-arylallyl cations (II) has been examined  
exptl. in strong acid solns. and theor. by HF/STO-3G calcns. The  
interconversions of I were intramol. processes in FSO<sub>3</sub>H, CF<sub>3</sub>SO<sub>3</sub>H, and  
FSO<sub>3</sub>H/SbF<sub>5</sub>. The rate consts. of the stereomutation of these cations, by  
dynamic NMR methods, depend on the substituents on the aryl ring. Apart  
from the case where the aryl ring bears two m-CF<sub>3</sub> groups, the rate consts.  
for stereomutation are linearly related to  $\sigma^+$  ( $\rho = -2.37$ ) with  
 $\pi$  donors accelerating the reaction. The calcns. performed for II show  
that the lowest energy pathway for isomerization involves rotation rather  
than inversion. They also reveal that  $\pi$ -donor substituents on the aryl  
ring lower the barrier to rotation while raising the barrier to inversion.  
In both cases, the calculated barriers for substituted systems show a linear  
correlation with  $\sigma^+$ . It is concluded that the preferred pathway for  
stereomutation of most of these 1-hydroxy- and 1-methoxyallyl cations in  
both strong acid solution and the gas phase involves rotation. When the aryl  
ring bears very strongly electron-withdrawing groups, e.g., two CF<sub>3</sub>  
groups, the inversion pathway seems preferred. This is the first example  
of a methoxycarbenium ion which undergoes stereomutation by inversion  
rather than rotation.

L7 ANSWER 7 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN

AN 1972:59617 CAPLUS

DN 76:59617

TI Alkyl esters of 1-(disubstituted phenyl or benzyl)-1H-indazol-3-  
yloxyacetic acids

IN Ambrus, Laszlo

PA Cutter Laboratories, Inc.

SO U.S., 5 pp.

CODEN: USXXAM

DT Patent

LA English

FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 3625971	A	19711207	US 1968-721937	19680417
	IL 31952	A	19730330	IL 1969-31952	19690402
	GB 1223945	A	19710303	GB 1969-1223945	19690416
	CH 514593	A	19711031	CH 1969-514593	19690417

PRAI US 1968-721937 A 19680417

GI For diagram(s), see printed CA Issue.

AB The title compds. (I, R=Cl or H; R1=H or CF3; R2=Et, Me, Pr, Bu, Bu-tert, or CH2CH2NEt2; n=0 or 1), useful as antiinflammatory agents (limb volume test in rats), were prepared by a Williamson ether synthesis. Thus, a mixture of 17 g 1-[3,5-bis(trifluoromethyl)phenyl]-1H-indazol-3-ol and 3 g MeONa in 200 ml MeCN and 50 ml EtOH was refluxed, 9 g BrCH2CO2Et, added in 1 hr, and the product refluxed 2 hr to give 14 g Et [1-[3,5-bis(trifluoromethyl)phenyl]-1H-indazol-3-yloxy]acetate (II). II had a lower oral toxicity when administered to rats than the corresponding acid. Six addnl. I were similarly prepared 2-(Diethylamino)-ethyl [1-[3,5-bis(trifluoromethyl)phenyl]-1H-indazol-3-yloxy]-acetate was prepared by treating 1-[3,5-bis(trifluoromethyl)-phenyl]-1H-indazol-3-yloxy)acetic acid with 2-(diethylamino)-ethyl chloride in iso-PrOH.

L7 ANSWER 8 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN

AN 1972:59616 CAPLUS

DN 76:59616

TI 1-(Disubstituted phenyl or benzyl)-1H-indazol-3-yloxyacetic acids

IN Ambrus, Laszlo

PA Cutter Laboratories, Inc.

SO U.S., 4 pp.

CODEN: USXXAM

DT Patent

LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 3625970	A	19711207	US 1968-721918	19680417
PRAI	US 1968-721918	A	19680417		

GI For diagram(s), see printed CA Issue.

AB The title compds. (I, R=Cl or H, R1=H or CF3, n=1 or 0), useful as antiinflammatory agents, were prepared by a Williamson ether synthesis. Thus, a mixture of 17 g 1-[3,5-bis(trifluoromethyl)phenyl]-1H-indazol-3-ol and 3 g MeONa in 200 ml MeCN and 50 ml EtOH was refluxed and 9 g BrCH2CO2Et was added in 1 hr. The product was refluxed 2 hr and saponified to give [1-(3,5-bis(trifluoromethyl)phenyl)-1H-indazol-3-yloxy]acetic acid (I, R=H, R1=CF3, n=0). I (R=2-Cl, R1=H, n=0) and I (R=H, R1=CF3, n=1) were similarly prepared. The acids exhibited antiinflammatory activity in rats when tested by the limb volume test.

L7 ANSWER 9 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN

AN 1971:449074 CAPLUS

DN 75:49074

TI Alkyl esters of 1-(disubstituted phenyl or benzyl)-1H-indazol-3-yloxy acetic acids

PA Cutter Laboratories, Inc.

SO Brit., 9 pp.

CODEN: BRXXAA

DT Patent

LA English

FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	GB 1223945	A	19710303	GB 1969-1223945	19690416
	US 3625971	A	19711207	US 1968-721937	19680417
PRAI	US 1968-721937	A	19680417		

GI For diagram(s), see printed CA Issue.

AB The title compds. (I) are derivs. of 1-(disubstituted-phenyl or benzyl)-1H-indazol-3-ols (II, R1 = CF3, R2 = CF3, halo, lower lower alkyl) in which the indazole nucleus has at its 3-position an ether O atom bearing a lower alkoxy carbonylmethyl group, CH2CO2R when R = lower alkyl optionally substituted by OH, alkoxy or dialkylamino. II are prepared by a series of reactions beginning with the phenylamine compound bearing the

R1,R2 substituents. The amine compound is acetylated and the acetamide arylated with PhBr, K<sub>2</sub>CO<sub>3</sub> and catalytic amts. of KI and CuBr in PhNO<sub>2</sub>. The resulting N-substituted acetamide is hydrolyzed with excess Cl<sub>2</sub>CO at -5 to +5°. The substituted carbamoyl chloride is treated with NaN<sub>3</sub> and the azide decomposition rearranged, and cyclized in refluxing xylene gives II. The title compds. are obtained by the Williamson ether synthesis by reaction of an alkali metal salt of II with an alkyl haloacetate in an inert solvent. Thus 17 g II (R1 = 3-CF<sub>3</sub>, R2 = 5-CF<sub>3</sub>) and 3 g NaOMe refluxed 1 hr in 200 ml MeCN and 50 ml alc. with addition of 9 g BrCH<sub>2</sub>CO<sub>2</sub>Et and the refluxing continued 2 hr gave Et [1-[3,5-bis(trifluoromethyl)phenyl]-1-H-indazol-3-yloxy]acetate. Similarly were produced seven other I. Substituted benzyl halides prepared by the Grignard reaction reacted with the mixture resulting from the reaction of an alkali metal alkoxide and indazolone give 1-benzyl-1H-indazol-3-ol. Thus 3,5-(F<sub>3</sub>C)<sub>2</sub>C<sub>6</sub>H<sub>3</sub>CH<sub>2</sub>Br, added to indazole and NaOMe in refluxing alc. and the concentrated mixture diluted with H<sub>2</sub>O gave

1-[3,5-bis(trifluoromethyl)benzyl]-1H-indazol-3-ol. I exhibit antiinflammatory activity and are useful as optical brighteners for use in detergent formulations.

=> s 16 and paraformaldehyde

17521 PARAFORMALDEHYDE

L8 1 L6 AND PARAFORMALDEHYDE

=> d bib abs

L8 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2007 ACS on STN

AN 2005:346966 CAPLUS

DN 142:392168

TI Grignard reaction process for the preparation 3,5-bis(trifluoromethyl)benzyl alcohol from 3,5-bis(trifluoromethyl)phenylmagnesium halides and solid paraformaldehyde

IN Nardello, Alessandro; Pretto, Marisa; Faccin, Andrea

PA Miteni S.p.A., Italy

SO PCT Int. Appl., 14 pp.

CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2005035472	A1	20050421	WO 2003-IT616	20031013
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	AU 2003279541	A1	20050427	AU 2003-279541	20031013
	EP 1673329	A1	20060628	EP 2003-772649	20031013
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, SK				
	US 2007135662	A1	20070614	US 2006-575485	20060707
PRAI	WO 2003-IT616	A	20031013		

OS CASREACT 142:392168

AB A Grignard reaction process for the preparation 3,5-bis(trifluoromethyl)benzyl alc. (I) from 3,5-bis(trifluoromethyl)phenylmagnesium halides [e.g., 3,5-bis(trifluoromethyl)phenylmagnesium bromide] and solid paraformaldehyde is described. I can then be converted into



3,5-bis(trifluoromethyl)benzyl halides [e.g., 3,5-bis(trifluoromethyl)benzyl bromide] by halogenation with hydrogen halides (e.g., hydrogen bromide).

RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> s 16 and grignard

44070 GRIGNARD

L9 2 L6 AND GRIGNARD

=> d 1-2 bib abs

L9 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2007 ACS on STN

AN 2005:346966 CAPLUS

DN 142:392168

TI Grignard reaction process for the preparation

3,5-bis(trifluoromethyl)benzyl alcohol from 3,5-

bis(trifluoromethyl)phenylmagnesium halides and solid paraformaldehyde

IN Nardello, Alessandro; Pretto, Marisa; Faccin, Andrea

PA Miteni S.p.A., Italy

SO PCT Int. Appl., 14 pp.

CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2005035472	A1	20050421	WO 2003-IT616	20031013
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	AU 2003279541	A1	20050427	AU 2003-279541	20031013
	EP 1673329	A1	20060628	EP 2003-772649	20031013
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, SK				
	US 2007135662	A1	20070614	US 2006-575485	20060707
PRAI	WO 2003-IT616	A	20031013		

OS CASREACT 142:392168

AB A Grignard reaction process for the preparation 3,5-bis(trifluoromethyl)benzyl alc. (I) from 3,5-bis(trifluoromethyl)phenylmagnesium halides [e.g., 3,5-bis(trifluoromethyl)phenylmagnesium bromide] and solid paraformaldehyde is described. I can then be converted into 3,5-bis(trifluoromethyl)benzyl halides [e.g., 3,5-bis(trifluoromethyl)benzyl bromide] by halogenation with hydrogen halides (e.g., hydrogen bromide).

RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2007 ACS on STN

AN 1971:449074 CAPLUS

DN 75:49074

TI Alkyl esters of 1-(disubstituted phenyl or benzyl)-1H-indazol-3-yloxy acetic acids

PA Cutter Laboratories, Inc.

SO Brit., 9 pp.

CODEN: BRXXAA

DT Patent  
LA English  
FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	GB 1223945	A	19710303	GB 1969-1223945	19690416
	US 3625971	A	19711207	US 1968-721937	19680417
PRAI	US 1968-721937	A	19680417		

GI For diagram(s), see printed CA Issue.

AB The title compds. (I) are derivs. of 1-(disubstituted-phenyl or benzyl)-1H-indazol-3-ols (II, R1 = CF3, R2 = CF3, halo, lower lower alkyl) in which the indazole nucleus has at its 3-position an ether O atom bearing a lower alkoxy carbonylmethyl group, CH2CO2R when R = lower alkyl optionally substituted by OH, alkoxy or dialkylamino. II are prepared by a series of reactions beginning with the phenylamine compound bearing the R1,R2 substituents. The amine compound is acetylated and the acetamide arylated with PhBr, K2CO3 and catalytic amts. of KI and CuBr in PhNO2. The resulting N-substituted acetamide is hydrolyzed with excess Cl2CO at -5 to +5°. The substituted carbamoyl chloride is treated with NaN3 and the azide decomposition rearranged, and cyclized in refluxing xylene gives II. The title compds. are obtained by the Williamson ether synthesis by reaction of an alkali metal salt of II with an alkyl haloacetate in an inert solvent. Thus 17 g II (R1 = 3-CF3, R2 = 5-CF3) and 3 g NaOMe refluxed 1 hr in 200 ml MeCN and 50 ml alc. with addition of 9 g BrCH2CO2Et and the refluxing continued 2 hr gave Et [1-[3,5-bis(trifluoromethyl)phenyl]-1-H-indazol-3-yloxy]acetate. Similarly were produced seven other I. Substituted benzyl halides prepared by the Grignard reaction reacted with the mixture resulting from the reaction of an alkali metal alkoxide and indazolone give 1-benzyl-1H-indazol-3-ol. Thus 3,5-(F3C)2C6H3CH2Br, added to indazole and NaOMe in refluxing alc. and the concentrated mixture diluted with H2O gave 1-[3,5-bis(trifluoromethyl)benzyl]-1H-indazol-3-ol. I exhibit antiinflammatory activity and are useful as optical brighteners for use in detergent formulations.